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Baroi, G. N.; Gavala, Hariklia N.; Westermann, P.; Skiadas, Ioannis

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Corresponding Author: Dr. Ioannis V. Skiadas, PhD

Corresponding Author's Institution: Technical University of Denmark

First Author: George Baroi

Order of Authors: George Baroi; Hariklia Gavala; Peter Westermann; Ioannis V. Skiadas, PhD

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Highlights (for review)

- High yield of butyrate (0.45 g g^{-1} sugar) can be achieved from fermentation of wheat straw
- In-situ acids separation by electro dialysis is necessary to secure high yields
- Butyrate production from straw is economically viable for big enough plant capacities
- The optimum plant capacity lies between 10 and 15 million kg of product per year
- Estimated unit production cost is around 3 $/kg and payback time less than 5 years

Fermentative production of butyric acid from wheat straw: economic evaluation

G.N. Baroi[a], H.N. Gavala[b], P. Westermann[a] and I.V.Skiadas[b,*]

[a]Aalborg University, Department of Chemistry and Bioscience, A C Meyers Vænge 15, DK 2450 Copenhagen SV, Denmark

[b]Technical University of Denmark, Department of Chemical and Biochemical Engineering, Søltofts Plads Bldg 228, 2800 Kgs. Lyngby, Denmark

[*]*Corresponding author: e-mail: ivsk@kt.dtu.dk & ioannis_sk@yahoo.co.uk, tel: +4545252729.*

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Key words: Economic analysis, Wheat straw, Butyric acid, Fermentation, C. tyrobutyricum, Electrodialysis

1. Introduction

Butyric acid is a four carbon fatty acid, which is commonly found in milk and milk products such as butter and has diverse applications in food and feed, chemical and pharmaceutical industries (Dwidar et al., 2012). In the chemical industry, the primary application of butyric acid is plastic production (e.g. cellulose-acetate-butyrate) (Cao et al., 2011). Previous research has also shown that butyric acid can be converted to butanol in a two steps fermentation process where sugars are converted to butyric acid in the first step by *C. tyrobutyricum* and in the second (solventogenic) step, butyric acid is converted to butanol by *C. acetobutylicum* (Ramey, 1998). The current annual production of butyric acid is estimated to be around 50,000 tonnes (Sauer et al., 2008) and it is mainly produced by oxidation of butyraldehyde (obtained from propylene derived from crude oil by oxosynthesis). Currently, the chemical synthesis of butyric acid is preferred mainly because of its lower production cost and the availability of the starting materials (Dwidar et al., 2012). Due to the increasing petroleum prices (in the long term), the concerns about greenhouse gas emission and global warming and the customers' preferences, butyric acid production from renewable resources is receiving growing interest from the scientific community and the industry (Zhang et al., 2009; Zigova and Sturdik, 2000) . However, biological production of butyric acid (e.g. from lignocellulosic biomasses) is relatively costly (Dwidar et al., 2012) and petroleum based production cannot be economically outcompeted by the renewable alternatives so far.

Wheat straw is the most abundant agricultural biomass in the world after rice straw (Kim and Dale, 2004) with, approximately, 600 million tonnes of wheat straw produced globally in 2009 (estimation based on FAO grain production data) (Bakker et al., 2013). Agricultural biomass is extensively exploited for production of power and biofuels. Particularly, in India, agricultural residues (e.g. rice husk, small wood chips, rice husks, cotton stalks, and other agro-residues) are used for grid power generation but the major

portion of agricultural biomass (e.g straw) is currently left in the fields (Mangaraj and Kulkarni, 2011). However, recent actions encouraged by the governmental policy supporting a low-carbon growth path increased potential exploitation of agricultural biomass (Purohit and Fischer, 2014).

Typical process for biological production of butyric acid from lignocellulosic biomasses such as wheat straw comprises pre-treatment, saccharification, fermentation, extraction and purification. Pre-treatment and enzymatic hydrolysis (saccharification), in general, is similar to 2G ethanol production process (Kazi et al., 2010) with weak acid hydrolysis being one of the most common pretreatment methods also for fermentative butyric acid production (Jha et al., 2014). Fermentation and acids extraction processes have been discussed in several review articles where different in-situ extraction strategies including solvent extraction and electrodialysis were suggested (Dwidar et al., 2012; Zhang et al., 2009; Zigova and Sturdik, 2000). Typical solvent extraction methods tested so far include physical extraction, reactive extraction or pertraction using different solvents such as decanol, and alamine 336/oleyl-alcohol with the main disadvantage being their inhibitory effect on the fermentation process. Recently, Baroi et al. (2015) reported promising results from a butyric acid production method based on the fermentation of pre-treated and enzymatically hydrolyzed wheat straw (PHWS), which was successfully tested in laboratory as well as in pilot scale. In this method, a single strain (*C. tyrobutyricum*, which cannot hydrolyse cellulose or hemicellulose) fermentation process was applied in combination with in-situ acids separation by Reverse Electro Enhanced Dialysis (REED). This resulted at a high butyric acid productivity, yield and selectivity (1.30 g L^{-1} h^{-1}, 0.45 g g^{-1} sugar, and 0.88 g g^{-1} acids respectively) which was accompanied by significantly smaller (but not negligible) acetic acid production. One possibility to eliminate acetic acid in the fermentation step is using a co-

culture of symbiotic microbial species (methanogens), which are able to convert acetic acid and hydrogen (released by butyric acid producing bacteria) to methane but are not able to consume butyric acid and have similar growth requirements with *C. tyrobutyricum*. This microbial symbiotic relationship is very common and naturally occurs in anaerobic digestion processes (Batstone et al., 2002). Metahnogens such as *Methanosarcina sp* and*Methanosaeta sp.* can catabolize H_2-CO_2 and acetic acid, respectively (Stams et al., 2003). It is expected that a co-culture of *C. tyrobutyricum* with methanogens will obviously have the advantage of resulting in a fermentation broth containing only butyric acid and (practically) no acetic acid with additional production of methane (which could be used as fuel for the process). On the other hand, the fermentation step will have to be designed for a longer hydraulic retention time in order to avoid washing out of the methanogens which grow slower than *C. tyrobutyricum*(Khanal, 2008).

To our knowledge, the above mentioned butyric acid efficiency is the highest observed so far in suspended growth fermentation systems and therefore, it is worthy to further examine possibilities for upscaling and commercial exploitation. Techno-economic analysis is a fundamental tool for studying the feasibility of new processes and estimating their economic viability and performance. A representative software package which is commercially available and can be used for simulation and techno-economic analysis of processes is SuperPro Designer®. SuperPro Designer® has among others been used for the techno-economic analysis of bioethanol production (Kazi et al., 2010; Wooley et al., 2002), bio-diesel production (Marchetti et al., 2008) and biopharmaceutical process optimization (Petrides et al., 2014) by estimating mass and energy balances as well as economic parameters. Furthermore, SuperPro Designer® can provide the distribution of cost over different process sections and perform cash flow analysis.

In the present study, a complete plant is envisaged where wheat straw is pretreated, enzymatically hydrolyzed and fermented to butyric acid, which is subsequently separated by applying the process developed by Baroi et al. (2015). The plant, which is assumed to have a production capacity of around 10,000 tonnes purified acids as main product (MP) from wheat straw, is analyzed and simulated by SuperPro Designer®, technoeconomic analysis is performed and its economic feasibility is evaluated.

2. Methods

2.1 Description of the process model

The process model includes five major process steps: feedstock handling, pretreatment, saccharification, fermentation and extraction and purification (see figure 1). The detailed process model, developed by using SuperPro Designer® V9.0, is shown in figure 2. In addition to the five sections, the model includes heat and power generation units where by-products such as solids and biogas are used for steam and power generation. Feedstock handling includes size reduction, which in combination with pretreatment facilitates the disintegration of the lignocellulosic structure of the biomass and thus increases the release of sugar monomers in the saccharification step. The liquid fraction of the latter step is then used for butyric acid fermentation. Organic acids produced in the fermentation step are extracted by distillation in the final purification step.

Figure 1 here

In most of the single strain fermentation processes developed so far for butyric acid production acetic acid is a side product even after genetic modification (Zhu et al., 2005). Acetic acid is also produced during the pretreatment. Butyric acid purification technologies after extraction are not yet fully developed and often butyric acid is produced as a mixture

(Zigova and Ernest, S, Vandak D, 1999). Acetic acid (boiling point 117.95 ^{0}C) has an almost similar pKa value as butyric acid (boiling point 164.85 ^{0}C) and both acids form azeotropic mixtures with water making the purification energy demanding. Hence, two scenarios (S1 and S2) were investigated in this study. S1 is based on the fermentation process developed by Baroi et al. (2015) where a mixture of butyric acid with acetic acid is the main product (MP). S2 is based on the same bacterium used in S1 (*C. tyrobutyricum*) in coculture with methanogens, which are able to convert acetic acid to methane and thus butyric acid is the MP. Each of the scenarios is modelled in SuperPro Designer where materials and energy balances are developed and then used for the economic evaluation of the processes.

Figure 2 here

2.1.1 Feed stock

Composition, availability and thus prices of wheat straw can vary significantly depending on the climate, soil and harvesting time as well as local market conditions (Molinuevo-Salces et al., 2013). As a result, unit production costs can be affected by these parameters when wheat straw is used as feedstock. In 2009-2010, wheat and rice straw production in India reached 186 million tonnes and 75% of this was either burnt or wasted (Mangaraj and Kulkarni, 2011). Furthermore, prices of wheat straw in India (0.0125 $/kg (Mangaraj and Kulkarni, 2011)) are considerably lower than in Denmark and Sweden (0.0724 $/kg (Statistik, 2014) and 0.108 $/kg (Horváth et al., 2013)) Due to large availability and very low prices of straw it is assumed that the plant for butyric acid production from wheat straw considered in the present study will be located in India. Hence, this study considers India as a potential ground for this process.

Major constituents of wheat straw are cellulose, hemicellulose and lignin as shown in table 1. Furthermore, wheat straw contains silica as 13% to 18% of ash content (Antongiovanni and Sargentini, 1991; Halvarsson et al., 2010) and 8 to 14% water (Bauer et al., 2009; Larsen et al., 2012) . The chemical composition of wheat straw used in this study was assumed to be cellulose 39.7%, hemicellulose 23.9%, lignin 20.5% and ash 5.7% as averages of the respective values presented in table 1.

Table 1 here

2.1.2 Feedstock handling and pre-treatment

Feedstock handling includes wheat straw washing and size reduction. Fresh water requirement in this process is assumed to be minimal since water generated in downstream purification steps is used in the washing step. Washed straw is passed through a grinder for size reduction down to 2-3 mm increasing the surface area, which facilitates the subsequent physicochemical pre-treatment step (Njoku et al., 2012). Storage cost is not taken into account for the estimation of unit production cost in this study.

The primary objective of the pretreatment is to make the carbohydrates, imbedded in lignocellulosic biomass, accessible for enzymatic hydrolysis (saccharification) (Galbe and Zacchi, 2002; Taherzadeh and Karimi, 2008). In the process considered in the present study, washed and grinded straw is transferred to the pretreatment reactor where it undergoes wet explosion (reactions outlined in table 2) followed by pressure release and temperature drop to 1 bar and 32 ^{0}C respectively in a flash tank. Wet explosion is carried out at 150 ^{0}C, retention time of 15 min, H_2SO_4 concentration of 0.3% (w/w), total solids (TS) content of 12-13% and a pressure of 6 bar (Biswas et al., 2013; Njoku et al., 2012). Heat released in this step is recycled to preheat the biomass feeding stream to the pretreatment reactor. The pretreated

straw is transferred from the flash tank to the saccharification step. For the purpose of the present study and in order to avoid the modelling of very complex commercial scale pretreatment reactor design, for which there is not enough information available (Kumar and Murthy, 2011), the pretreatment step is assumed to be one piece of equipment shown in figure 2 (pretreatment reactor grouping together a series of equipment such as screw conveyors, tanks, reactor, flash tank etc.)

Table 2 here

2.1.3 Saccharification

The slurry, produced after the pretreatment, has a very low pH (<5.0) and therefore, prior to enzymatic hydrolysis, pH is adjusted to 5 by adding NaOH. Enzyme complex dose (Cellic CTec2), reaction temperature, and residence time are 50 g/kg cellulose, 30^0C and 24 hours respectively (Öhrman et al., 2013). Reactions and conversion efficiency used in saccharification modeling are shown in table 2. After saccharification, the remaining solids are separated by a belt-filter as suggested by Wooley et al. (2002). During this filtration step, water is used for washing purposes at so small quantities that it may be assumed as negligible without introducing significant error in the overall process modelling and calculations. The separated solid fraction, usually called ‘cake’, is characterized by a moisture content of 50% and is used for heat and power generation. The remaining liquid stream is utilized as the substrate for the following fermentation step.

2.1.4 Fermentation coupled with extraction

Prior to fermentation, the liquid is neutralized with potassium hydroxide, and urea and K_2HPO_4 are added at a concentration of 4.5 g/L and 0.64 g/L respectively. The mixture is then

sterilized at a temperature of 140 ^{0}C and pumped into the fermentation tank. For both scenarios (S1 and S2) examined in this study the fermentation is carried out at a temperature of 37 ^{0}C and pH 7 following the fermentation stoichiometry and conversion efficiencies presented in table 2. The hydraulic retention time (HRT) is not assumed the same in the two scenarios. As demonstrated by Baroi et al., (2015), recommended HRT for scenario S1 is 1.28 d. However, the maximum specific growth rate for methanogens is between 0.25 and 0.5 d^{-1} (Gavala et al., 2003) which corresponds to a minimum HRT between 2 and 4 d for the methanogens to grow fast enough and not being washed out. Thus the HRT for scenario S2 is assumed to be 2 d. *C. tyrobutyricum,* which is assumed in this study, has previously been well adapted to the fermentation medium (wheat straw hydrolysate) (Baroi et al., 2015; Baroi et al., 2015a) and therefore, is not expected to be affected by any inhibition. On the other hand, methanogens may be inhibited by compounds in wheat straw hydrolysate(Shanmugam et al., 2014). Based on literature data, it is assumed here that this inhibition effect is not severe and also that adaptation of the methanogens will take place and thus the longer hydraulic retention time used in S2 will be sufficient to maintaining a healthy methanogens population in the fermentation system (Rivard and Grohmann, 1991).

For both S1 and S2 scenarios the fermentor is connected with a membrane system for in-situ separation of butyric acid. Specifically, the fermentation broth flows through a REED anion-exchange membrane unit where organic acid anions (e.g. $CH_3(CH_2)COO^-$) are removed from the broth facilitated by an electric field and replaced by OH^- coming from a NaOH solution flowing at the opposite side of the membrane. The organic acid anions are then combined with the remaining Na^+ and the formed salt solution is passed through an EDBM (electrodialysis with bipolar membrane) unit which regenerates the NaOH and releases a water solution of the organic acids as demonstrated by (Garde, 2002; Wang et al., 2013). In

this process, there is a loss of a small part of NaOH, which is replenished by an external addition of a NaOH solution. Butyric acid and acetic acid recovery efficiencies for the REED unit are 90% and 91% respectively as reported by Baroi et al. (2015). Organic acids recovery efficiency of EDBM is assumed to be 100% which is similar to that used by Garde (2002) for lactic acid production. Based on estimations made by Jurag Separation A/S, the providers of REED/EDBM technology, the butyric acid content of the acid solution generated by the EDBM unit was expected to be around 5.5%. In the present study, the REED/EDBM units are modeled as one unit for simplification purposes. Detailed operational parameters and technical characteristics of REED/EDBM are presented in table 3. Finally, the effluent from the fermentation tank (from which organic acids have been removed and recovered) is assumed to be wastewater that requires proper treatment and disposal.

Table 3 here

2.1.5 Purification

The purification steps include storage, extraction and distillation units. 1-octanol (as a representative model solvent) was selected for the extraction of organic acids from the water phase coming from the REED/EDBM unit. The partition co-efficient (PC) of butyric acid in octanol was 6.17 and the PC of acetic acid was 0.68. The solubility or entrainment of water in octanol or octanol in water was assumed 0.01 g/L. After extraction, the octanol phase that contains the organic acids is distilled. The organic acids (butyric and acetic acids for S1 or only butyric acid for S2), which are more volatile than octanol are collected from the top of the distillation column as the main product while octanol leaves from the bottom of the distillation vat and is recycled back to the extraction unit after replenishment of the octanol losses. Detailed operational parameters and technical characteristics of extraction and

distillation units are presented in table 3. The distillation processes were modelled in SuperPro Designer® using a semi-empirical shortcut method (Fenske-Underwood-Gilliland). The distillation column is operated at a reflux ratio of 41 and 48 for S1 and S2 respectively. Heat recovered from the distillation effluent streams is used for pre-heating the feed stream. The water phase from the bottom of the extraction unit is used as washing water in the straw washing unit and finally ends up as wastewater that requires proper treatment and disposal.

2.1.6 Combined heat and power (CHP) generation

The filter cake, which is produced during belt filtration of hydrolyzed straw as well as the biogas from the fermentation unit are combusted for heat and power production where well water is used for steam generation. It is assumed that the steam and electricity produced in this step are fully consumed by the modelled enterprise to cover energy needs of the rest of the process steps. Detail operating parameters for CHP are presented in table 3, There is a possibility to tune parameter in SuperproDesigner® to get different pressure steam in order to satisfy the needs of the production process. However, default values were chosen for steam generator.

2.2 Economic analysis

The economic evaluation of butyric acid production from wheat straw studied in the present work involved the estimation of capital cost, variable and fixed operating costs as well as profitability. SuperPro Designer® was used in order to model and simulate the production process. The calculated material and energy balances were then used for equipment sizing and cost estimation. The purchase costs for some of the equipment (such as belt filtration, sterilization unit, extraction, distillation unit, steam generation unit, heat exchangers and

coolers) were obtained from SuperPro Designer® existing databases combined with the build-in scaling law (equation 1) while for others (such as washing table, shredder, pretreatment vessel, flush tank, enzymatic hydrolysis, fermentation reactor, storage tanks, REED and EDBM) the purchase costs calculations were based on the simulated equipment sizes and the application of scaling law with specific equipment index taken from previous reports (Aden et al., 2002; Garde, 2002).

$$New\ Cost\ = \text{Original Cost}\ \left(\frac{New\ Size}{Orizinal\ Size}\right)^{n} \quad (1)$$

Where n=specific equipment index

Additionally, SuperPro Designer® accounted for the cost of secondary equipment, which was not listed for model simplification purposes. The purchase cost of this unlisted equipment was estimated to be 20% of the purchase cost of listed equipment. Finally and as recommended by SuperPro Designer®, maintenance cost was assumed to be 10% of the total equipment purchase cost. Equipment, raw materials and labor purchase costs which are subject to changes with time due to inflation and other parameters influencing market conditions were estimated by equation 2, where specific indexes are used to estimate the purchase cost for the desired year (Cost2) when the cost is known for a previous year (Cost 1):

$$Cost2\ = \text{Cost1}\ \frac{Index_2}{Index_1} \quad (2)$$

The necessary parameters for the estimation of the total capital investment cost and operating cost of the process were obtained from literature (Humbird et al., 2011; Ou et al., 2014). Thus, the project life and the depreciation period were taken as 20 and 10 years respectively while

the salvage value, the construction and start-up period and the inflation rate were 5%, 30 months, 6 months and 4% respectively.

2.2.1 *Raw materials, consumables, utilities, labor and waste disposal costs*

The prices of raw materials used in the present process modeling and economic evaluation are shown in table 4. Where necessary, the prices have been adjusted by indexing them to year 2014 as suggested by Aden et al. (Aden et al., 2002). The price of wheat straw used as feedstock in this study was 0.0125 $/kg (see also section 2.1.1 Feedstock). Octanol price varied from 1.65-1.83 $/kg but an average value of 1.7 $/kg was used in this study. Also, it was assumed that the enzyme prices would remain stable during the years included in the evaluation even though one can expect lowering prices due to future technological development. Prices of consumables such as membranes used for REED (198 $/$m^2$) and EDBM (1567 $/$m^2$) were taken from Garde (2002) and adjusted for the year 2014 using equation 2. Purchase costs of utilities such as water (0.203 $/tonne), electricity (0.07 $/kWh) and steam (115^{0}C , 60.95 $/tonne) as well as labor price (basic 2.5 $/h) are taken from literature (Burkley, 2014; Sikder et al., 2012) and, where necessary, they were adjusted for the year 2014. It is remarkable though, that steam price in India seemed several times higher compared to what has been reported in other similar studies for ethanol production (17.08 $/tonne (year 2006 price) (Kwiatkowski et al., 2006)) or biogas production (4.05 $/tonne (year 2013 price) (Shafiei et al., 2013)). The above are the buy-in prices of energy utilities, if the CHP does not satisfy demand.

The cost for wastewater treatment and disposal can vary significantly depending on its organic load (BOD or COD content). Harrison et al. (2013) reported a disposal fee of 0.2 $/$m^3$ to 0.5 $/$m^3$ for waste water having a BOD content less than 1000 mg/L which was

the expected organic load of the effluent from wheat straw wash unit. However, the wastewater mixture generated during the present butyric acid production process, that is the fermentation effluent mixed with the effluent from straw wash unit, was expected to have significantly higher organic load. Buyukkamaci and Koken, (2010) estimated a cost of 0.7-2.35 $/m^3 for the treatment of high strength (10 g COD/L and 5 g/L suspended solids) paper and pulp industry wastewater. Garde (2002) used a cost of 2.36 $/m^3 for the treatment of wastewater from a fermentative lactic acid production process. The cost for wastewater (both fermentation effluent and washing water) treatment assumed in this study was 2 $/m^3. Finally, the cost for the disposal of the ash generated in the heat and power section was assumed to be at 0.0041 $/kg (Wooley et al., 2002). The costs of the waste/wastewater treatment and disposal are not necessarily representative of those in India. These costs are bound to vary considerably across municipalities, and even more so across continents. However, these costs are usually a very small portion of the total operating cost and it is assumed in the present study that they cannot influence significantly the economics of the examined production process. This assumption is confirmed from the results of the present study presented below in section 3.2. Furthermore, the used costs are representative of North Europe and North America which (due to very strict environmental regulations) present the highest costs compared to other geographical areas and thus the economic evaluation results of the present study cannot be influenced negatively by locating the production unit in India.

Table 4 here

2.2.2 *Product price*

Current market price of butyric acid was not possible to be recovered from public databases. However, butyric acid price can be estimated from the price of n-butyraldehyde, which is the

raw material used during the chemical synthesis of butyric acid. Zidwick et. al. (2013) reported a butyric acid price of 1.5 $/kg in year 1982 based on the market price of n-butyraldehyde. Since then, there has been a considerable increase of oil price, which has resulted to significant increases of butyric acid price reported by producers such as EASTMAN (www.eastman.com) or OXEA (www.oxea-chemicals.com). Recently, OXEA has reported a list price of n-butyraldehyde at 3.95 $/kg (OXEA, 2014) and thus list price of butyric acid can be be 4.78$/kg (production cost factor of 1.21 was calculated based on the data reported by Zidwick et al. (2013)). However, due to the uncertainties with the above price estimations it has been chosen a minimum price for butyric acid of 3.95 $/kg being the same with that of n-butyraldehyde. Thus the economic evaluation was performed on a worst case scenario where the price of butyric acid produced through chemical synthesis will be so low as this of n-butyraldehyde. The purity of the commercially available butyric acid varies from 99 to 99.5%. In order to perform cash flow analysis in this study the price of butyric acid (purity >99%) was assumed to be 3.95 $/kg. The main product resulting from scenario S1 is a mixture of butyric acid and acetic acid. Butyric acid content in this mixture is 89%. Based on a 89% purity of butyric acid, the price of the product from S1 was assumed to be 3.50 $/kg, calculated proportionally from the price used for the product with 99 % purity. The product from S2 was assumed to be pure (99%) butyric acid.

2.3 *Parameters for Sensitivity analysis*

Depending on local conditions and their yearly variation, such as climate, yield of crops, and feedstock availability versus demand, the price of feedstock (wheat straw) may have a large variation and thus affect substantially the unit production cost. In order to demonstrate the effect of wheat straw price as well as that of plant size (capacity) and selling price of main

product on the profitability of the whole enterprise, a sensitivity analysis was performed (single parameter at a time) by using SuperPro Designer® Component Object Model (COM) interface in combination with Microsoft Excel® interface.

3. Results and Discussion:

3.1 Economic summary of the scenario S1 and S2

The economic results for plant product capacity of 10,000 tonnes per year after simulation of both S1 and S2 scenarios are presented in tables 5 and 6. Based on a market price (year 2014) estimation for butyric acid at 3.95 $/kg (purity 99%) both scenarios showed encouraging results. Unit production cost was estimated at 2.75 $/kg product and 3.31 $/kg product for S1 and S2 respectively. For the plant capacity examined in this study (10,000 tonnes of product per year) this reveals a very efficient investment with Internal Rate of Return (after tax) of 14.92% and 12.42 % and payback time of 4.28 and 4.7 years for S1 and S2 respectively.

Total Lang factors (Peters and Timmerhaus, 1991) of 5.07 and 5.10 were used for S1 and S2 respectively to estimate total capital investment based on equipment purchase cost. This estimation resulted in a total capital investment for scenarios S1 and S2 of 47.71 and 53.68 million $ respectively. Due to the conversion of acetic acid to methane in S2, S1 results in higher amount of MP produced per unit amount of straw consumed and thus S1 is required to convert a smaller amount of wheat straw(140 tonnes compared to 156 tonnes per day) in order to produce 10,000 tonnes of MP per year. Consequently, the equipment size in S1 is slightly smaller than in S2 and accordingly the estimated capital investment for S1 is smaller than for S2. In order to test how realistic are the above estimated capital investments a comparison with the results from a similar study by Humbird et al. (2011) was made. This comparison revealed that for the same raw material capacity used by Humbird et al. (i.e. 2,000 tonnes of

raw material per day) S1 and S2 would require a total capital investment of 410,652,000 $ and 426,090,000$ respectively which is almost the same with the 422,500,000 $ estimated by Humbird et al. Operating cost was slightly higher for S2 (33.12 million $) compared with S1 (27.52 million $) scenario which (after taking into consideration that butyric acid purity for S1 and S2 was 89 % and 99 % respectively) resulted in an increased (20%) unit production cost for scenario S2. A small amount of credit was obtained due to electricity and steam generation in the heat and power section (figure 3a) and this has resulted to a 16% reduction of the unit production cost.

Figure 3 here

Table 5 here

Table 6 here

Direct Fixed Capital Cost and its breakdown to different cost categories are shown in table 6. Estimated *Direct Fixed Capital Cost* for S1 and S2 is 40.32 and 45.07 million $ respectively. The highest equipment purchase cost was attributed to the pretreatment section (26%) followed by fermentation and extraction section (22%) and purification section (21%). Detailed equipment costs and respective size or capacity of each unit are presented in appendix A.

3.2 Operating cost distribution for scenarios S1 and S2

The different operating cost categories for scenarios S1 and S2 are shown in table 7. Utility costs are the highest (52.7% and 55.0 % of the total operating cost for S1 and S2 respectively) followed by facility dependent costs (28.4 % and 26.36%) and raw material costs (8.1% and 7.6%). Facility dependent costs include maintenance, deprecation and miscellaneous costs.

Operating costs distributed among the six sections of the process are shown in figure 3b. For both S1 and S2 scenarios, purification section was the most costly one accounting for ~50 % of the total operating cost. Fermentation accounted for ~ 26%, pretreatment ~11 %, saccharification ~5.5 % and feed stock handling ~ 4% for both S1 and S2.

The operating costs of the purification section was estimated at 13.62 and 17.12 million $ for S1 and S2 respectively. This means that the purification section accounted for more than 80% of the total utility costs followed by fermentation and separation (15%), heat and power section (~ 2%) and pretreatment (~ 1%). As mentioned above, steam is relatively expensive in India and thus, steam alone contributed to 34.2 % and 35.8% of the total operating cost of S1 and S2 respectively (table 7). A large amount of steam (154,419 tonnes for S1 and 194,274 tonnes for S2) and cooling water (12.83 million tonnes for S1 and 16.16 million tonnes for S2) were used by the process. However, 46.7% (S1) and 44.4 % (S2) of the total steam demand could in principle be covered by the CHP unit (see figure 3a).

The operating cost of fermentation and separation section was estimated at 7.5 and 8.5 million $ (for S1 and S2 respectively), of which, utility costs were approximately 33%. A significant amount of electricity was required for REED and EDBM units. Total electricity purchase cost for the entire plant was estimated at 2.4 and 2.8 million $. Almost 95% of the electricity consumption of the entire plant was used in fermentation and separation section. Total electricity consumption by S1 and S2 was 34.4 and 39.4 GWh/year respectively. However, a very small amount of electricity (0.35 and 0.38% of the total plant consumption for scenario S1 and S2) is generated by the CHP section.

The cost of replacement of REED and EDBM membranes corresponded to approximately 20% of the operating cost of fermentation and separation section. Among the different raw materials used, urea (as nitrogen source for microbes) was the most costly and

corresponded to almost 2.5% of the total operating costs. Costs for wheat straw, NaOH and enzymes were significant but not as high. The total amount of wheat straw necessary for the production of 10,000 tonnes MP from S1 and S2 was 44,060 and 49,820 tonnes respectively.

Table 7 here

3.3 Sensitivity analysis

Sensitivity analysis was performed to determine the potential effect of wheat straw prices on the unit production cost for scenarios S1 and S2 and the results are shown in figure 4a. A hypothetical increase of 1000% in the purchase price of feedstock may cause an 80% increase in production cost for S1 and S2, indicating that in general feedstock price has a minor effect . This result could be explained by the fact that, in the specific case handled in the present study, wheat straw purchase cost (0.01 $/kg) contributed with a relatively small percentage to the total operating cost. Apparently, this cost increment may not be significant under the assumptions of the present study but it is likely that this picture will change in the future due to lower availability of wheat straw as a result of, for example, installation of a number of wheat straw based production plants or low crops efficiency, due to climate change. Furthermore, wheat straw prices may have had a more significant impact on the unit production cost if the necessary heat and power were produced through the combustion of wheat straw together with the produced biogas and solid cake. However and according to our knowledge, similar phenomena have not been observed for another biomass type and, thus, this alternative was not taken into consideration during the present sensitivity analysis.

Figure 4 here

The effect of plant size (capacity) on the unit production cost as well as revenue, net profit, return of investment (ROI) and internal rate of return (IRR) for S1 and S2 may be seen

in figures 4b and 5. The unit production costs decrease nonlinearly with increasing plant size. The unit production cost increase sharply with plant sizes less than 10,000 tonnes MP/year while it is not affected significantly (the curve is almost flat) for plant sizes higher than 15,000 tonnes MP/year implying that a plant with a production capacity smaller than 10,000 tonnes MP per year would most probably be a very weak choice. This is clearly supported also from the investment performance indexes (ROI and IRR) presented in figure 5 where both ROI and IRR decrease sharply for plant sizes smaller than 10,000 tonnes MP /year for S1 as well as for S2. While profit keeps increasing linearly with plant size, ROI and IRR follow a rather different behavior where an increase of plant size above 10,000-15,000 tonnes MP/year results to a disproportional smaller increase of these indexes. Given the fact that the present economic evaluation has not taken into consideration the possible limitations with wheat straw availability for large scale plants which could result in deterioration of these indexes, one could conclude that a reasonable plant size would lie between 10,000 and 15,000 tonnes MP/year with an IRR (after tax) around 16%.

Figure 5 here

Payback time decreases and IRR increases when the selling price of the product increases. The payback time for a plant with a capacity of 10,000 tonnes MP per year with selling price of 3.50 and 3.95 $/kg MP was estimated at 4.28 and 4.70 years for scenarios S1 and S2 respectively (see figure 6). When the selling price of MP was less than 2.8 $/kg for S1 and 3.2 $/kg for S2, IRR became zero and the investment could not be paid back. Thus one can conclude that the above prices are the minimum MP celling prices for a plant with a capacity of 10,000 tonnes MP per year.

Figure 6 here

3.3 Alternative approach for heat and power production

As it is evident from the figures in table 7, utility cost for both scenarios S1 and S2 became quite high mainly due to the high purchase cost of steam. Therefore, instead of purchasing steam, one could generate the necessary process steam in the plant's heat and power section where wheat straw or rice straw or both, depending on the availability, could be combusted for steam generation. As it can be seen in table 8, this would of course result in an increased raw materials purchase cost (an additional 69100 tonnes/yr and 84800 tonnes /yr wheat straw would be necessary for S1 and S2 respectively) and cost of heat and power section but it would also considerably decrease the utility cost. Thus the total operating cost would be lower and finally it would have been possible to operate the plant at the same capacity but at a lower unit production cost. For example, if wheat straw alone was used for the generation of the process steam required for the production of 10,000 tonnes MP per year, operating cost could be reduced by 33 and 35 % and, similarly, unit production cost could be reduced to 1.84 and 2.16 $/kg MP for S1 and S2 respectively (table 8). It needs to be mentioned here that, in the present study, the butyric acid is meant as a commodity chemical and not as a fuel and, as such, its production will always demand some external energy supplies. This production can of course be pushed to a more sustainable direction if the external energy (e.g. electricity) can be supplied by renewable sources such as wind or solar energy instead of fossil resources.

Table 8 here

Conclusions

A wheat straw based plant with a butyric acid production capacity of 10,000 tonnes per year through pretreatment, enzymatic hydrolysis, fermentation and in-situ membrane extraction

was envisaged and economically evaluated in the present study. The plant design and economic evaluation was based on processes simulation using SuperPro Designer® V9.0 software. The hypothetical plant was chosen to be located in India where the feedstock purchase cost was found to be very low. Two different scenarios (S1 and S2) of fermentative butyric acid production from wheat straw were developed and evaluated in this work. Scenario S1 resulted in the production of butyric acid (89% purity) in mixture with acetic acid and scenario S2 resulted in the production of butyric acid of 99% purity. The higher product purity from scenario S2 was not enough for improving the economy of the process since the utilities demand per unit of processed feedstock remained approximately the same and more feedstock had to be handled in order to result at the same annual production capacity as S1. Feedstock (wheat straw) purchase cost, which was relatively very small, was not found to have any substantial impact on the economic efficiency of the plant. On the contrary, utilities were the most decisive cost parameter mainly due to the consumption of relatively expensive steam in the purification (distillation) section. When the selling price of butyric acid was less than 2.8 $/kg for S1 and 3.2 $/kg for S2, IRR became zero and the investment could not be paid back. Thus, one can conclude that the above prices are the minimum MP selling prices for a plant with a capacity of 10,000 tonnes product per year. An alternative in-house steam production through straw combustion could decrease the unit production cost down to 1.84 and 2.16 $/kg of product for S1 and S2 respectively. Increasing plant size had a positive effect on revenue and profit but could not significantly increase IRR. Given the fact that the present study has not taken into consideration the possible limitations with wheat straw availability and the resulting increase of feedstock purchase cost for large scale plants, a reasonable plant size would lie between 10,000 and 15,000 tonnes of product per year.

Process flow diagrams for the two scenarios studied (S1 and S2) built on SuperPro Designer® V9.0 platform are provided as supplementary material. Binary plots of 1-octanol and butyrate and acetate are presented in the appendix

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Table 1. Major components of wheat straw as percentage of dry matter.

Polymers	(Petersen et al., 2009)	(Hansen et al., 2013)	(Georgieva et al., 2008)
Cellulose	35.0	42.3	41.8
Hemicellulose	22.3	24.0	25.3
Lignin	15.6	22.4	23.4
Ash	6.5	5.1	5.6
Others	20.9	Not reported	Not reported

Table 2: Stoichiometry of reactions and conversion efficiency assumed for the different unit processes involved in the present process model.

Reactions	**Fraction (%) converted to product**
Pretreatment (Wet Explosion)	
Cellulose + 1.11 H_2O → 1.11 Glucose	6.00
Cellulose → HMF + 3H_2O	0.09
Hemicellulose + 0.136 H_2O → 1.136 Xylose	61.56
Hemicellulose + 0.136 H_2O → 1.136 Arabinose	4.44
Hemicellulose → 0.64 Furfural + 0.36 H_2O	1.14
Enzymatic hydrolysis	
Cellulose + 1.11 H_2O → 1.11 Glucose	85.00
Hemicellulose + 0.136 H_2O → 1.136 Xylose	60.00
Fermentation	
Glucose + 0.63 Xylose → 0.24 Acetic acid + 1.47 Butyric acid + 2.79 CO_2 + 2.64 H_2 + 0.14 H_2O	100
Methanogenesis	
Acetate → Methane + CO_2	100
Hydrogen + CO_2 → Methane + H_2O	100

Table 3: Detailed operational parameters and technical characteristics of the unit operations and processes used in this model.

Unit Name	Type	Material of Construction	Details
WSH-101	Washer	CS	Silica removal efficiency >99%
SR-101	Shredder	CS	0.01 kW/(kg/h) Specific power
V-105	Sulfuric acid storage tank	SS316	Residence time 5 days, working to vessel volume ratio 90%
GP-101	Gear pump to transport straw into pretreatment reactor	SS316	Pressure change 5 bar, power efficiency 70%
PFR-102	Pretreatment reactor	SS316	Residence time 15 min, temperature 150 ^{0}C, total solids 15% specific power 0.1kW/m^3
V-101	Flash drum	CS	Pressure 1bar, residence time 5 min, work to vessel volume ration 60%, temperature 30^{0}C
V-107	PH cotrol before saccharification	CS	residence time 0.5h, 0.1 kW/(kg/h) Specific power, 0.01% excess NaOH
V-106	Enzyme tank	SS316	Residence time 5 days, working to vessel volume ratio 90%
R-101	Sccarification reactor	SS316	Residence time 24h, temperature 32^{0}C, specific power 0.1kW/m3, total solids 15%, working to vessel volume ratio 90%
BF-101	Belt filter for soilds seperation	CS	Solids in cake 50%, flow per unit belt width 10L/min-m, solids loading 3000 (kg/h)/m
V-104	Neutralizer	CS	residence time 0.5h, 0.1 kW/(kg/h) Specific power, 0.01% excess KOH
ST-101	Heat sterilizer	SS316	Sterilization temperature 140^{0}C, exit temperature 41^{0}C
R-102	Fermentation reactor	SS316	Residence time 1.28 (for S2) and 2 (for S1) days, temperature 37^{0}C, specific power 0.1kW/m^3, working to vessel volume ratio 90%, effluent split 0.88% of the total recirculation
V-108	Dialyzate tank	SS316	Residence time 1 day, working to vessel volume ratio 90%
G2	REED+EDBM	CS	REED (power 0.1547 kW/(kg/h), current efficiency 0.7, current density 500A/m^2, average recovery 92%); EDBM (power 0.1547 kW/(kg/h), current efficiency 0.72, current density 1000A/m^2, average recovery 100%), butyric acid final concentration 5.5%
V-103	Acid storage tank	SS316	Residence time 2h, working to vessel volume ratio 90%
MSX-101	Mixer-settler extractor	SS316	Mixer residence time 0.5h, settler residence time 1h, temperature 32 ^{0}C, specific power

			0.5kW/(kg/h)
C-101	Distillation column	CS	Number of stages 25, Reboiler temperature 175^0C, condenser temperature 165^0C, column pressure 1bar, max dia 2 m, stage height 0.4m
PM-101	Boiler feed water pump	SS316	Pressure change 94 bar, power efficiency 70%
SG-101	Steam generator	CS	Excess oxygen 10%, overall heat loss 5%, flue gas exit temperature 120 ^{0}C
T-101	Steam turbine	CS	Power generator efficiency 90 % of shaft power, 3 stages (high pressure steam 180^0C, low pressure steam 150^0C and bleed)

1

2

1

2 Table 4. Raw material prices used in this model.

Item Name	Price[a]	Unit	Reference
Wheat straw	0.0125	$/kg	(Mangaraj and Kulkarni, 2011)
Enzyme	0.571	$/kg	(Kumar and Murthy, 2011)
Sulfuric acid	0.035	$/kg	(Kumar and Murthy, 2011)
NaOH	0.45	$/kg	(Kumar and Murthy, 2011)
KOH	0.189	$/kg	(Ljunggren et al., 2011)
Urea	0.649	$/kg	(Sánchez-Segado et al., 2012)
Phosphate	0.891	$/kg	(Sánchez-Segado et al., 2012)

[a] Conversion factor: 1 US$ =0.74 EUR

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Table 5: Summary of the economics and mass and energy requirements for scenarios S1 and S2

	S1	S2	Unit
Total Capital Investment	47.71	53.68	million $
Capital Investment Charged to this project (100%)	47.71	53.68	million $
Operating Cost	27.52	33.12	million $/yr
Credits	4.65	5.56	million $/yr
Net Operating Cost	22.87	27.56	million $/yr
Revenues	35.05	39.46	million $/yr
Unit Production Cost	2.75	3.31	$/kg MP
Net Unit Production Cost	2.29	2.76	$/kg MP
Unit Production Revenue	3.51	3.95	$/kg MP
Gross Margin	34.75	30.16	%
Return On Investment	23.35	21.28	%
Payback Time	4.28	4.7	years
IRR (After Taxes)	14.92	12.42	%
NPV (at 7.0% Interest)	28.56	21.11	million $
Cost Basis Annual Rate	10000.07	10000.04	tonnes MP/yr
Feed stock (wheat straw)	46150.21	51611.59	tonnes/yr
Efficiency (mass MP/mass wheat straw)	0.22	0.19	
Power (electricity) demand	34831.14	38960.81	MW-h/yr
Net steam demand	17553.71	19630.00	tonnes/yr
Net steam (high P) demand	162987.52	201139.12	tonnes/yr

MP = Total flow of acid or mixed acids as main product
IRR = Internal Rate of Return
NPV = Net Present Value

Table 6: Direct fixed cost summary (year 2014 prices in million $) for scenarios S1 and S2.

	S1	S2
A. Total Plant Direct Cost (TPDC) (physical cost)		
1. Equipment Purchase Cost	9.42	10.53
2. Installation	3.67	4.11
3. Process Piping	2.92	3.26
4. Instrumentation	2.45	2.74
5. Insulation	0.28	0.32
6. Electrical	0.94	1.05
7. Buildings	2.73	3.05
8. Yard Improvement	1.13	1.26
9. Auxiliary Facilities	4.71	5.27
B. Total Plant Indirect Cost (TPIC)		
10. Engineering	3.11	3.48
11. Construction	3.40	3.80
C. Total Plant Cost (TPC = TPDC+TPIC)	34.76	38.85
D. Contractor's Fee & Contingency (CFC)		
12. Contractor's Fee	1.74	1.93
13. Contingency	3.82	4.27
E. Direct Fixed Capital Cost (DFC = TPC+CFC)	40.32	45.07

Table 7: Annual operating costs (million $) distribution for an annual production of 10,000 tonnes MP for both scenarios (S1, S2) for the year 2014.

	S1	% of Total	S2	% of Total
Labor				
Operator	0.73	2.65%	1.07	3.23%
Raw Materials				
Enzyme mix	0.40	1.45%	0.46	1.39%
Wheat straw (86%DM)	0.55	2.00%	0.62	1.87%
KOH	0.002	0.01%	0.002	0.01%
Octanol,1	0.04	0.15%	0.05	0.15%
K_2HPO_4	0.14	0.51%	0.15	0.45%
NaOH	0.28	1.02%	0.32	0.97%
H_2SO_4	0.03	0.11%	0.03	0.09%
Urea	0.70	2.54%	0.80	2.42%
Water	0.07	0.25%	0.08	0.24%
Consumables				
EDBM membrane	0.68	2.47%	0.77	2.32%
Anion exchange membrane	0.36	1.31%	0.41	1.24%
Cation exchange membrane	0.42	1.53%	0.48	1.45%
NaOH‡	0.003	0.01%	0.003	0.01%
Waste Disposal				
Ash	0.04	0.15%	0.04	0.12%
Wash waste water	0.31	1.13%	0.35	1.06%
Effluent	0.34	1.24%	0.39	1.18%
Utility		0.00%		
Std Power	2.41	8.76%	2.76	8.33%
Steam	0.21	0.76%	0.23	0.69%
High Pressure steam	9.41	34.19%	11.84	35.75%
Cooling Water	2.61	9.48%	3.28	9.90%
Facility-Dependent	7.81	28.38%	8.73	26.36%
Laboratory/QC/QA	0.11	0.40%	0.16	0.48%
TOTAL	27.52		33.12	

‡ For the sake of calculation NaOH used in REED and EDBM system is considered as consumable

Table 8: Economic summary and operating cost distribution (year 2014) for S1 and S2 when considering in-house steam generation by CHP unit.

	S1	S2
Total Capital Investment (million$)	49.04	54.14
Operating Cost (million$)	19.34	22.99
Unit Production Cost ($/kgMP)	1.84	2.16
Direct Fixed Capital (million$)	42.53	47.24
Operating cost (2014 prices) summary (million$)		
Cost Item		
Raw Materials	2.62	3.04
Labor-Dependent	0.73	1.07
Depreciation	4.04	4.50
Other Facility-Dependent	4.20	4.66
Laboratory/QC/QA	0.11	0.16
Consumables	1.54	2.62
Waste Treatment/Disposal	0.75	0.87
Utilities	5.26	6.36
Total	19.24	23.27

APPENDIX A

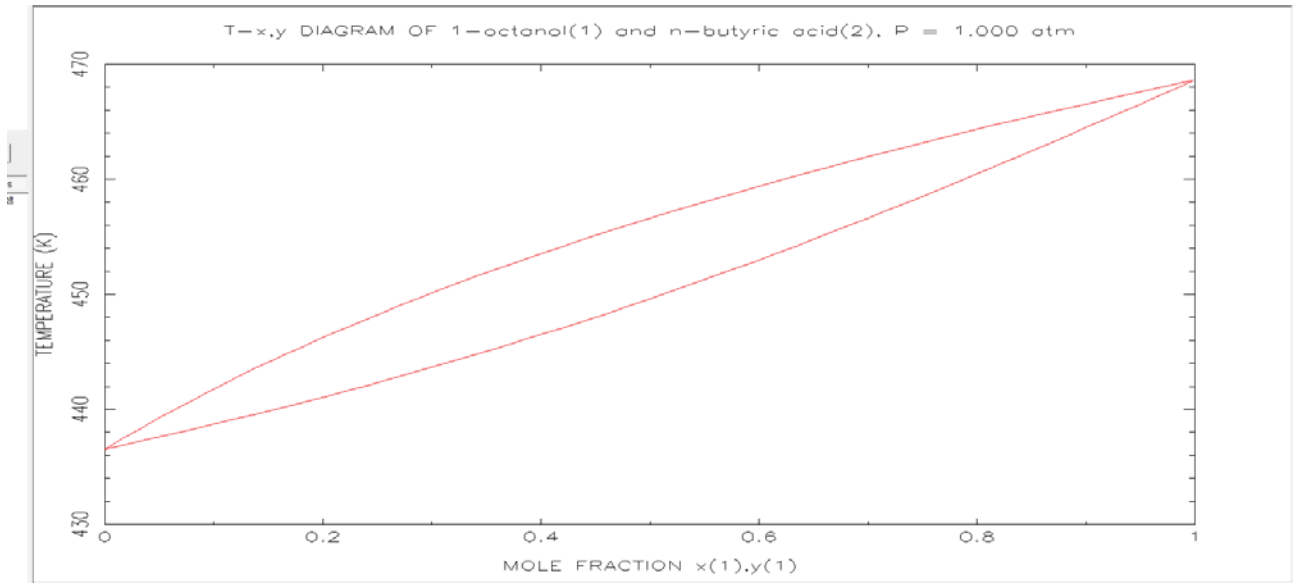
Table A1: Purchase cost (year 2014) and size or capacity of equipment unit used in this model for 10,000 tonnes MP production.

		S1	S2	S2
Name	Description	Cost ($)	Description	Cost ($)
Feed stock handling				
WSH-101	Washer (Bulk Flow)	1000	Washer (Bulk Flow)	1000
	Size/Capacity = 5.56 MT/h		Size/Capacity = 6.29 MT/h	
SR-101	Shredder	190000	Shredder	204000
	Size/Capacity = 5.52 MT/h		Size/Capacity = 6.24 MT/h	
Pretreatment				
V-105	Vertical-On-Legs Tank	22000	Vertical-On-Legs Tank	24000
	Vessel Volume = 7.12 m3		Vessel Volume = 8.05 m3	
GP-101	Gear Pump	16000	Gear Pump	18000
	Pump Power = 6.48 kW		Pump Power = 7.33 kW	
PFR-102	Plug Flow Reactor	286000	Plug Flow Reactor	308000
	Vessel Volume = 1.24 m3		Vessel Volume = 1.40 m3	
HX-104	Heat Exchanger	2032000	Heat Exchanger	2337000
	Heat Exchange Area = 99.60 m2		Heat Exchange Area = 94.83 m2	
V-101	Flash Drum	2000	Flash Drum	2000
	Vessel Volume = 4507.80 L		Vessel Volume = 5096.95 L	
Saccharification				
V-107	Neutralizer	89000	Neutralizer	95000
	Vessel Volume = 18.10 m3		Vessel Volume = 20.47 m3	
V-106	Vertical-On-Legs Tank	11000	Vertical-On-Legs Tank	12000
	Vessel Volume = 11.96 m3		Vessel Volume = 13.52 m3	
R-101	Stirred Reactor	355000	Stirred Reactor	382000
	Vessel Volume = 872.42 m3		Vessel Volume = 986.45 m3	
BF-101	Belt Filter	274000	Belt Filter	276000
	Belt Width = 0.54 m		Belt Width = 0.61 m	
Fermentation and seperation				
V-104	Neutralizer	84000	Neutralizer	90000
	Vessel Volume = 16.53 m3		Vessel Volume = 18.70 m3	
ST-101	Heat Sterilizer	722000	Heat Sterilizer	750000
	Rated Throughput = 29.89 m3/h		Rated Throughput = 33.80 m3/h	
R-102	Stirred Reactor	392000	Stirred Reactor	539000
	Vessel Volume = 1030.02 m3		Vessel Volume = 1746.89 m3	
V-108	Vertical-On-Legs Tank	165000	Vertical-On-Legs Tank	176000
	Vessel Volume = 353.49 m3		Vessel Volume = 401.63 m3	
REED+EDBM	Generic Box	695000	Generic Box	767000

	Size/Capacity = 20638.49 kg/h		Size/Capacity = 23339.16 kg/h	
Purification				
V-103	Flat Bottom Tank Vessel Volume = 46.46 m3	99000	Flat Bottom Tank Vessel Volume = 52.56 m3	102000
MSX-101	Mixer-Settler Extractor Rated Throughput = 154333.01 L/h	325000	Mixer-Settler Extractor Rated Throughput = 174515.94 L/h	350000
HX-102	Heat Exchanger Heat Exchange Area = 5.08 m2	21000	Heat Exchanger Heat Exchange Area = 5.29 m2	22000
HX-103	Heat Exchanger Heat Exchange Area = 91.02 m2	1200000	Heat Exchanger Heat Exchange Area = 96.02 m2	1364000
C-101	Distillation Column Column Volume = 50.99 m3	201000	Distillation Column Column Volume = 57.71 m3	212000
HX-101	Heat Exchanger Heat Exchange Area = 71.69 m2	104000	Heat Exchanger Heat Exchange Area = 80.17 m2	111000
Heat and power generation				
PM-101	Centrifugal Pump Pump Power = 3.71 kW	34000	Centrifugal Pump Pump Power = 4.44 kW	37000
SG-101	Steam Generator Throughput = 10116.47 kg/h	180000	Steam Generator Throughput = 12093.81 kg/h	206000
T-101	Multi-Stage Steam Turbine Turbine Delivered Shaft Power = 16.91 kW	37000	Multi-Stage Steam Turbine Turbine Delivered Shaft Power = 21.95 kW	39000
	Unlisted Equipment	1884000	Unlisted Equipment	2106000
	Total ($)	**9420000**		**10529000**

1

2



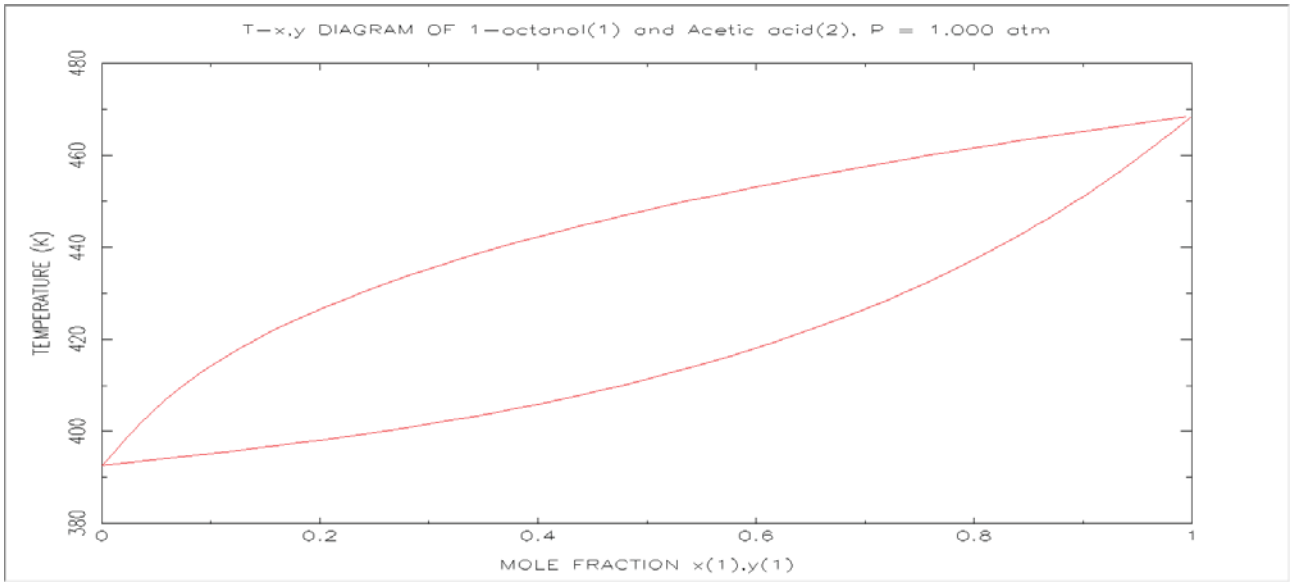


Figure A1. Binary phase diagrams for octanol/butyrate and octanol/acetate. No azeotrope formation is predicted. Thermodynamic model used included: equation of state, Soave-Redlich-Kwong; mixing rule, Modified Huron Vidal of 1st order; excess Gibbs energy model, UNIFAC VLE1.

Figure1

Figure 1: Process flow diagram showing different process steps

Figure2

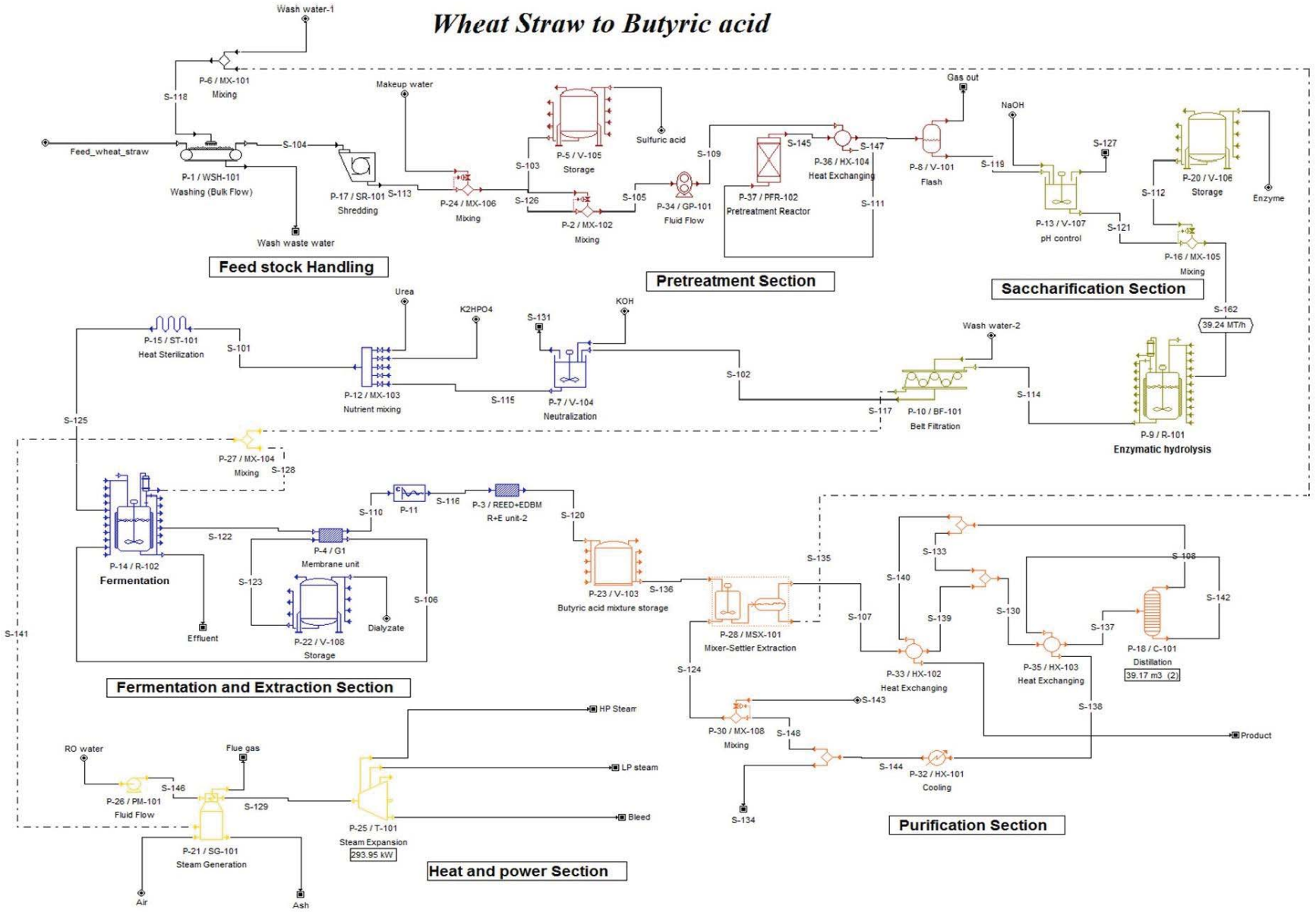


Figure 2: Process flow diagram for the production of acids from wheat straw.

Figure3

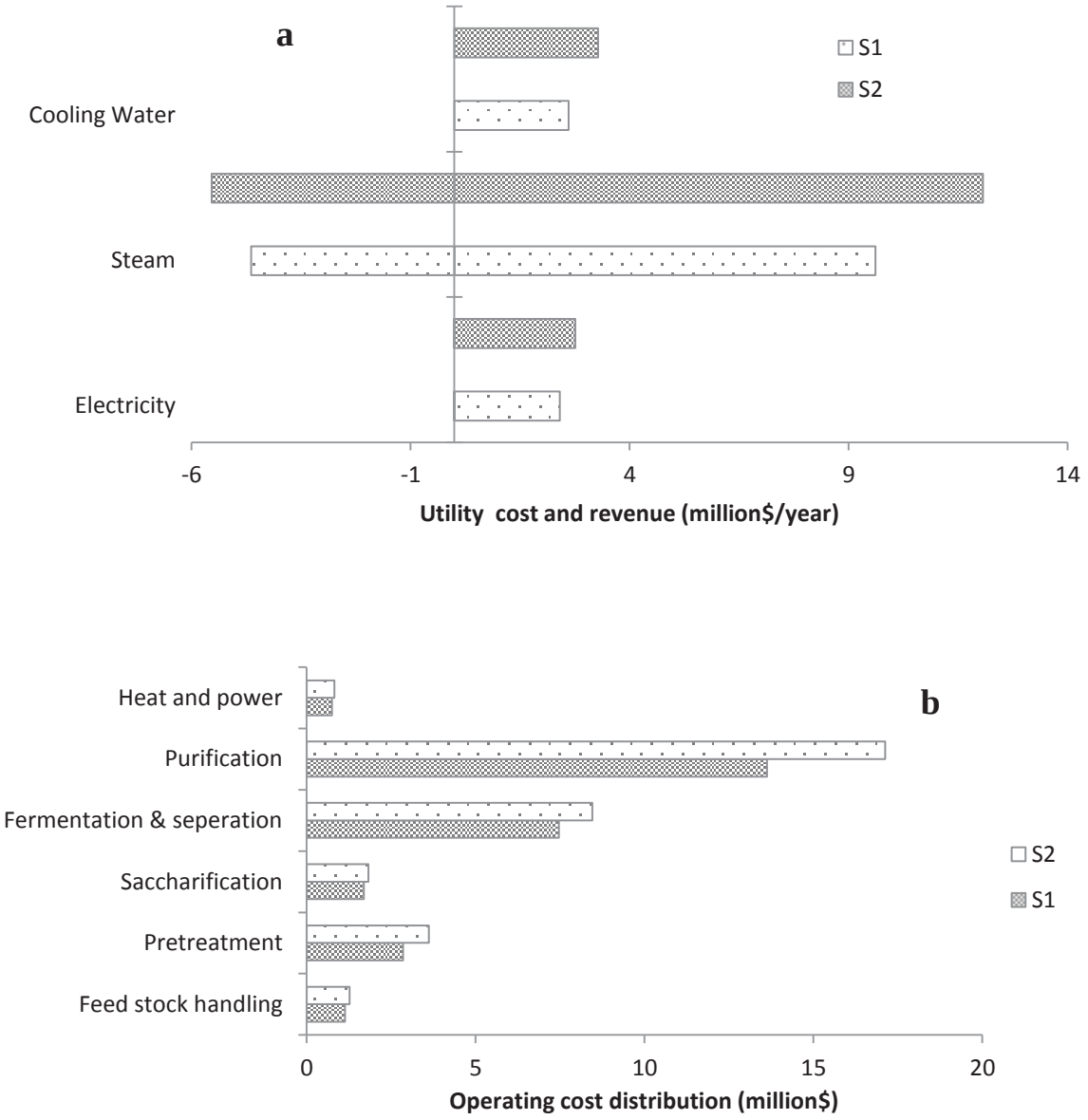
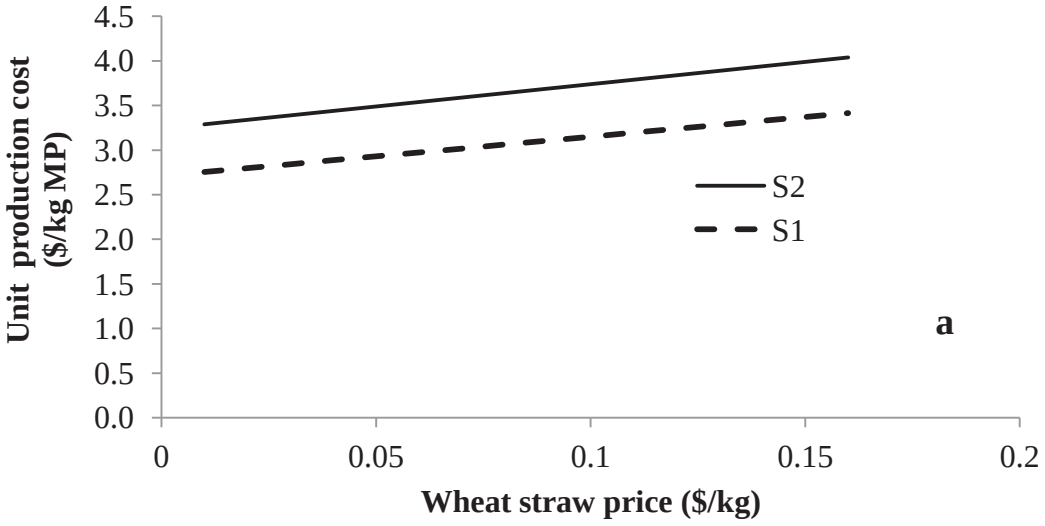


Figure 3: (a) Costs of utility and credit from heat and power section for both S1 and S2 scenarios. Credits are shown on the left side (negative) and costs are shown on the right side (positive). (b) Operating costs distributed among the six sections of the process and comparison between scenario S1 and S2.

Figure4



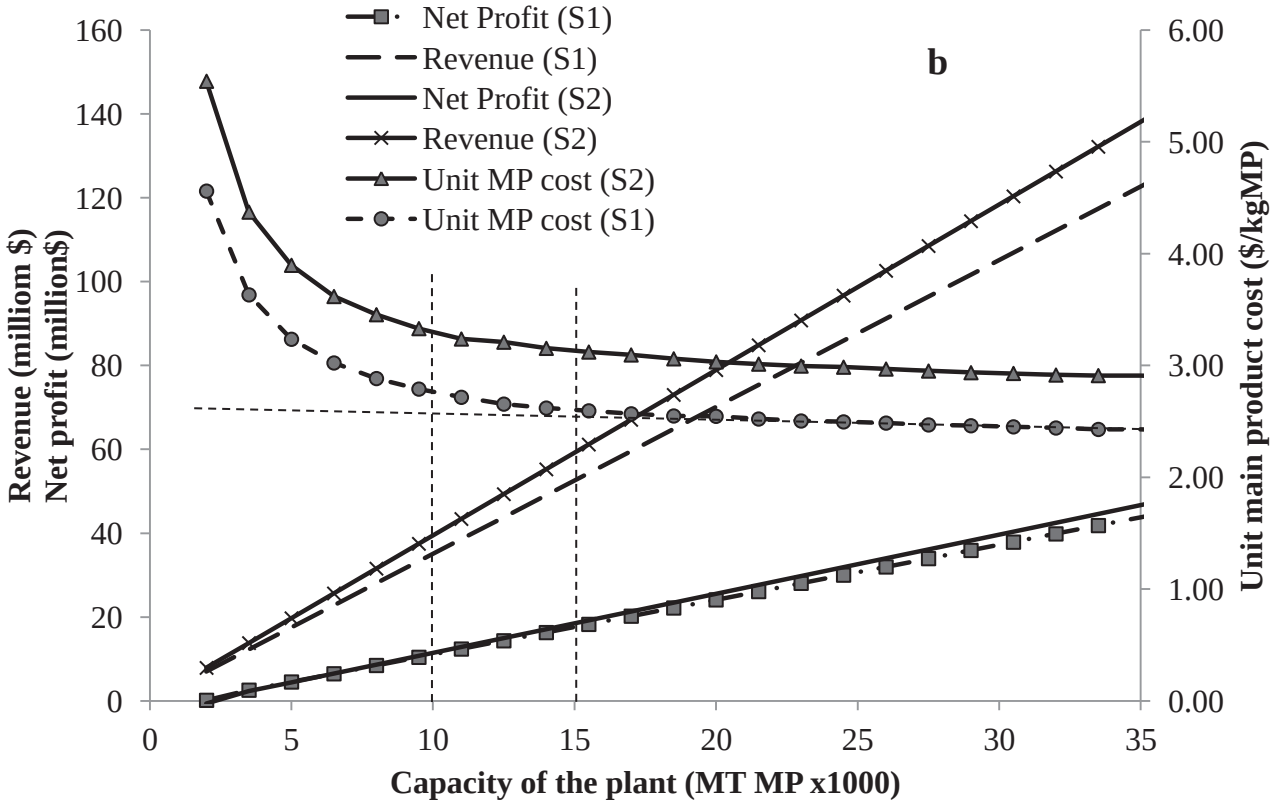


Figure 4: Effect of wheat straw price on unit production cost of MP (a) and effect of plant size on unit production cost of MP, revenue and net profit (b) for both S1 and S2 scenarios.

Figure5

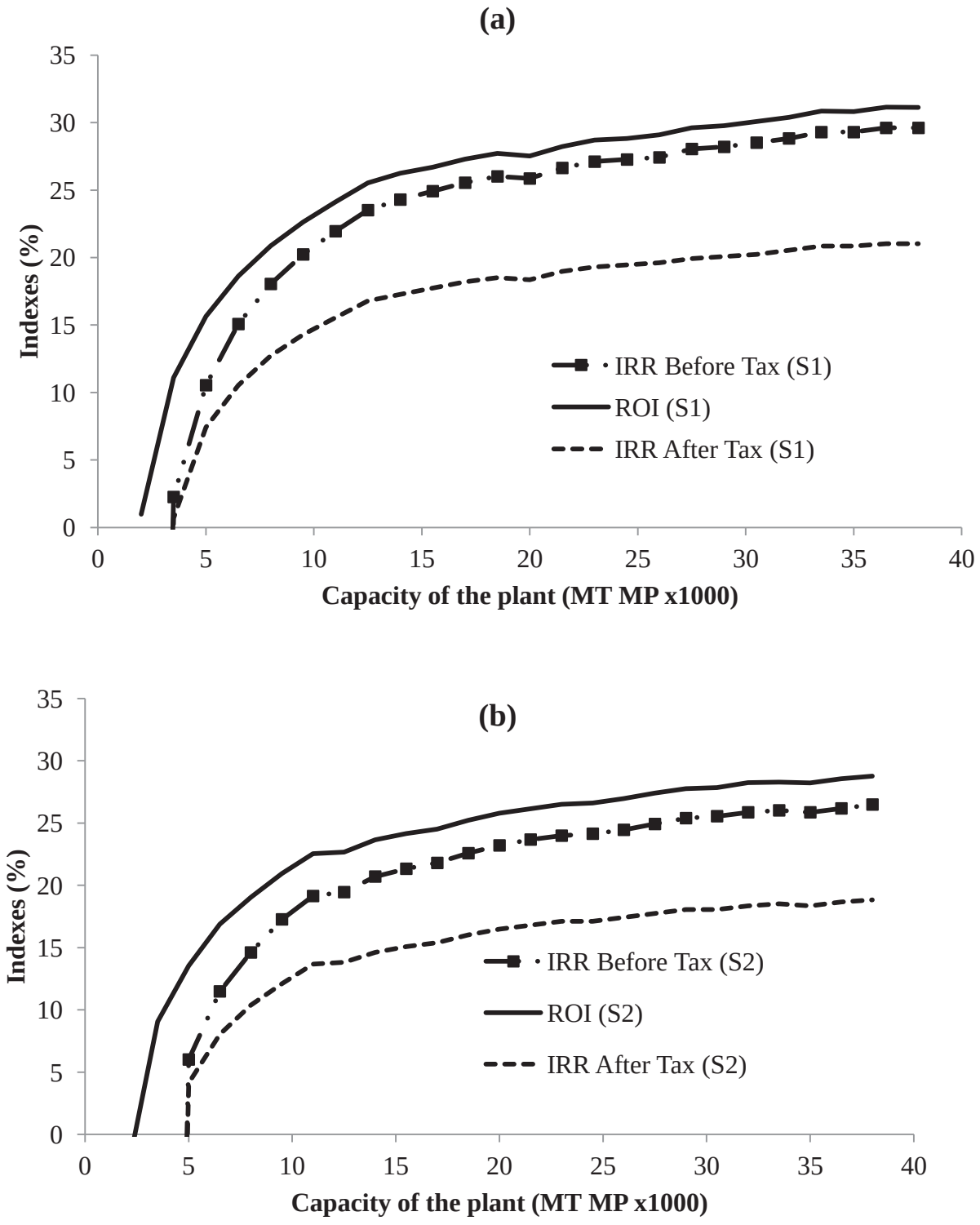


Figure 5: Effect of plant size on ROI and IRR before and after tax for scenario S1 (a) and scenario S2 (b).

Figure6

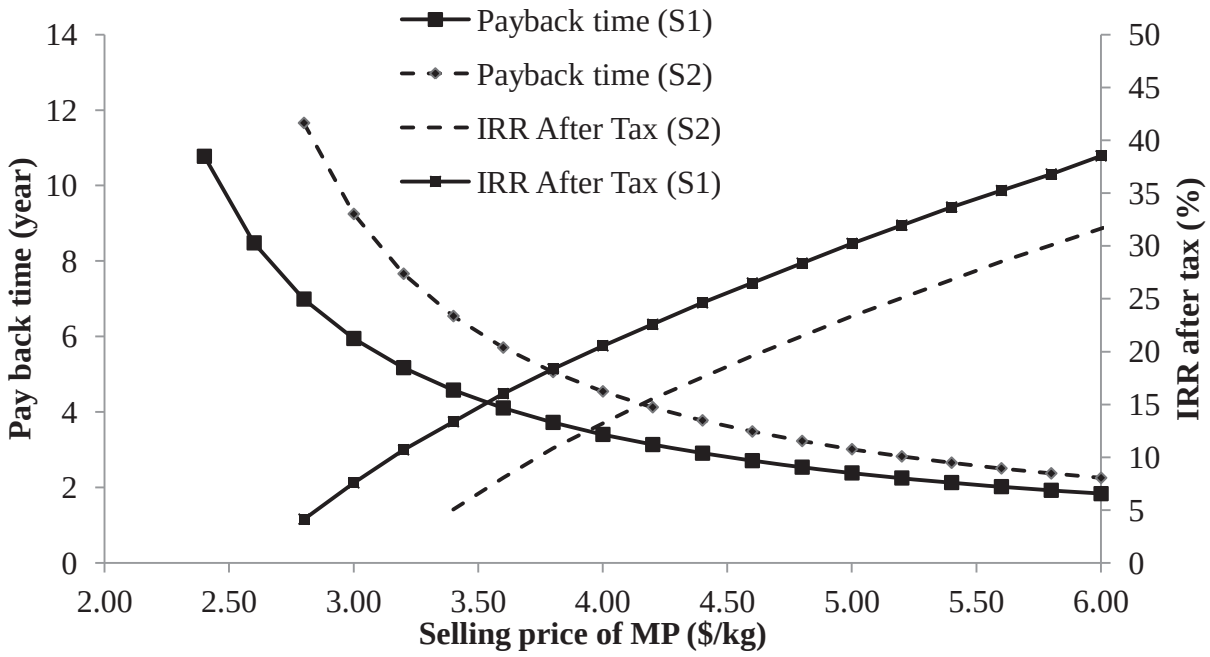


Figure 6: Effect of selling price of MP on payback time and IRR for both S1 and S2 scenarios for a plant with a capacity of 10,000 tonnes MP per year.

Figure Captions

Figure 1: Process flow diagram showing different process steps

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Process flow diagram of S1 in SuperPro Designer format

Click here to download Supplementary Interactive Plot Data (CSV): withoutmethane-1002-dp_octanol.spf

Process flow diagram of S2 in SuperPro Designer format

Click here to download Supplementary Interactive Plot Data (CSV): withmethane-1002-dp_octanol.spf